Coulomb Screening of 2D Massive Dirac Fermions

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A model of 2D massive Dirac fermions ,interacting with a instantaneous $1/r$ Coulomb interaction, is presented to mimic the physics of gapped graphene. The static polarization function is calculated explicitly to analyze screening effect at the finite temperature and density. Results are compared with the massless case . We also show that various other works can be reproduced within our model in a straightforward and unified manner.

PACS numbers: 05.30.Fk 71.10.-w 71 10.Ca

I. INTRODUCTION

Over the past several years, the physics of graphene has attracted considerable interest, both theoretically and experimentally[1]. Graphene, due to its two dimensional hexagonal lattice structure, has unique linear energy spectrum near the Dirac points of Brillouin zone. Because of the unusual energy band dispersion, many electronic properties in graphene exhibit significantly different behavior from the conventional 2D systems, for example, half-integer QHE(Quantum Hall Effect)[2].

In graphene although the motion of electrons are fixed on the 2D plane, their interactions still show 3D Coulomb's law, for the electric field lines cannot be confined on 2D. While most of the early work were based on massless Dirac fermion model, recent work has shown that the massive case can also be created[2].

For massive fermions, it is equivalent to the opening of a gap in the electronic spectrum in condensed matter physics. So the similarity between graphene and QED_{2+1} is obvious, and many results were obtained by exploring this correspondence[3]. While the main difference is that Graphene lacks of Lorenz invariance due to its nearly instantaneous coulomb interaction.

Besides, it should be noted there has been many papers [4][5][6][7] on the Coulomb interaction in gapless graphene. Ref.[4][5] gave the polarization function for zero temperature gapless graphene at finite density. Ref.[6] dealt with 2D Coulomb-interacting massless Dirac fermions and calculated the specific heat at finite temperature, while Ref.[7] generalized it to the finite density case. As for the massive Dirac fermions, there are also many work on it. However, most of them (gapless or gapped graphene) were highly succinct, used different models and did not give the calculations of polarization function in detail.

In this paper, we consider a model of two-component Dirac fermions interacting through a three dimensional instantaneous Coulomb interaction, and calculate the polarization functions at finite temperature and finite density using finite temperature field techniques[8]. In fact quantum field theory at finite temperature or density is usually applied to study cosmology and astrophysics But its 2D spatial case has not been observed in nature. So the graphene provides a wonderful platform for establishing QED_{2+1}. We also show various works on this topic can be connected within our model in a straightforward and unified manner.

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II. MODEL

Our starting point is a model of $2+1$ dimensional two-component Dirac fermions mediated by a three dimensional Coulomb interaction at temperature T. The action of the system S is given by ($\hbar = 1$)

$$\begin{aligned} S(\bar{\psi}, \psi, \varphi) \ = \ & \int_0^\beta d\tau \{ \int d^3x \frac{1}{8\pi} |\partial_i \varphi(x,\tau)|^2 + \int d^2x \sum_{s=1}^{N} \bar{\psi}_s(x,\tau)[\partial_\tau + v\boldsymbol{\sigma}\cdot\mathbf{p} + m\sigma_3 \\ & -\mu + ie\varphi(x,\tau)]\psi_s(x,\tau)\} \end{aligned} \tag{1}$$

Here, $\beta = 1/T$ and μ is the chemical potential. The fields ψ_s are two-component fermion fields, subscript index s stands for different species of fermions with $N = 4$ due to spin, valley degeneracies in graphene. The vector $\boldsymbol{\sigma} = (\sigma_1, \sigma_2)$ and $\sigma_i, i = 1,2,3$ are pauli matrices; $\sigma_0 = I$ is the 2×2 identity matrix(omitted for simplicity). φ is the field that mediates the Coulomb interaction, nothing but the time component of the electromagnetic field. The 3D space integral of the action describes the kinetic term of the scalar field, while the remaining terms describe kinetic term for the fermion fields and their interaction with the scalar field. In addition, we put $v = 1$ bellow and only restore it if necessary.

Correspondingly, the Green's function for the free Dirac fermions

$$G_0(k) = \frac{k_0 + \boldsymbol{\sigma}\cdot\mathbf{k} + m\sigma_3}{k_0^2 - \mathbf{k}^2 - m^2} \tag{2}$$

Using more symmetric three-momentum notation,$(q_0, \mathbf{q}) = (i\omega_l, \mathbf{q}), (k_0, \mathbf{k}) = (i\omega_n + \mu, \mathbf{k}), \tilde{k}^2 = k_0^2 - \mathbf{k}^2, \omega_n = (2n+1)\pi/\beta, \omega_l = 2l\pi/\beta$ etc.,then the polarization function in the random-phase approximation (RPA)[9] is

$$\begin{aligned} \Pi(q) &= \frac{4}{\beta}\sum_n \int \frac{d^2\mathbf{k}}{(2\pi)^2} Tr(G(\tilde{k})G(\tilde{k}+\tilde{q})) \\ &= \frac{8}{\beta}\sum_n \int \frac{d^2\mathbf{k}}{(2\pi)^2} \frac{k_0(k_0+q_0) + \mathbf{k}(\mathbf{k}+\mathbf{q}) + m^2}{(\tilde{k}^2 - m^2)[(\tilde{k}+\tilde{q})^2 - m^2]} \end{aligned} \tag{3}$$

where $v(\mathbf{q}) = 2\pi e^2/\kappa|\mathbf{q}|$ is the 2D Fourier transform of the 3D Coulomb interaction. Following similar consideration in Ref.[10] we can divide Π into two contributions, the vacuum part and matter part.

$$\Pi = \Pi_{vac} + \Pi_{matter} \tag{4}$$

$$\lim_{T\to 0, \mu\to 0} \Pi = \Pi_{vac} \tag{5}$$

The vacuum polarization function, both massless and massive case, can be calculated by dimensional regularization approach as in Ref.[3][12]. Here, we can reproduce their results within our model

$$\Pi_{vac}(q) = -\frac{|\mathbf{q}|^2}{\pi}\{\frac{m}{q^2} + \frac{1}{2q}(1 - \frac{4m^2}{q^2})\arctan(\frac{q}{2m})\} \tag{6}$$

III. POLARIZATION FUNCTION FOR MASSIVE DIRAC FERMIONS

The sum of fermion Matsubara frequencies can be performed in a standard manner[11].

$$
\begin{aligned}
&\frac{1}{\beta}\sum_n \frac{k_0(k_0+q_0)+\mathbf{k}\cdot(\mathbf{k}+\mathbf{q})+m^2}{(k_0^2-E_{\mathbf{k}}^2)[(k_0+q_0^2)-E_{\mathbf{k}+\mathbf{q}}^2]} \\
=& -\frac{1}{2\pi i}\oint dz h(z) g(z) \\
=& -\frac{1}{2\pi i}\int_{i\infty-\epsilon}^{-i\infty-\epsilon} dz h(z)\frac{1}{2}\tanh(\beta z/2) - \frac{1}{2\pi i}\int_{-i\infty+\epsilon}^{i\infty+\epsilon} dz h(z)\frac{1}{2}\tanh(\beta z/2) \\
=& -\frac{1}{2\pi i}\int_{i\infty-\epsilon}^{-i\infty-\epsilon} dz h(z)(\frac{1}{2}-\frac{1}{e^{-\beta z}+1}) - \frac{1}{2\pi i}\int_{-i\infty+\epsilon}^{i\infty+\epsilon} dz h(z)(-\frac{1}{2}+\frac{1}{e^{\beta z}+1})
\end{aligned} \tag{7}
$$

With

$$
h(z) = \frac{(z+\mu)(z+\mu+q_0)+\mathbf{k}\cdot(\mathbf{k}+\mathbf{q})+m^2}{[(z+\mu)^2-E_{\mathbf{k}}^2][(z+\mu+q_0^2)-E_{\mathbf{k}+\mathbf{q}}^2]}
$$

$$
g(z) = \frac{\beta}{2}\tanh(\beta z/2)
$$

$$
E_{\mathbf{k}} = \sqrt{\mathbf{k}^2+m^2}
$$

For function $g(z)$ has simple poles at $z = i\omega_n$, the sum emerge as the integration of the product hg along a suitable path in the complex plane. We can divide the above expressions into two parts π_{vac}, π_{matter}, which describe the vacuum and matter's contributions respectively.

$$
\pi_{vac} = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} dz[h(z)+h(-z)]/2 \tag{8}
$$

$$
\begin{aligned}
\pi_{matter} =& -\frac{1}{2\pi i}\int_{-i\infty+\epsilon}^{i\infty+\epsilon} dz h(z)\frac{1}{e^{\beta z}+1} + \frac{1}{2\pi i}\int_{i\infty-\epsilon}^{-i\infty-\epsilon} dz h(z)\frac{1}{e^{-\beta z}+1} \\
=& \frac{1}{2E_{\mathbf{k}}}\frac{E_{\mathbf{k}}(E_{\mathbf{k}}+q_0)+\mathbf{k}(\mathbf{k}+\mathbf{q})+m^2}{(E_{\mathbf{k}}+q_0)^2-E_{\mathbf{k}+\mathbf{q}}^2}\frac{1}{e^{\beta(E_{\mathbf{k}}+\mu)}+1} \\
&+\frac{1}{2E_{\mathbf{k}}}\frac{E_{\mathbf{k}}(E_{\mathbf{k}}-q_0)+\mathbf{k}(\mathbf{k}+\mathbf{q})+m^2}{(E_{\mathbf{k}}-q_0)^2-E_{\mathbf{k}+\mathbf{q}}^2}\frac{1}{e^{\beta(E_{\mathbf{k}}-\mu)}+1} \\
&+\frac{1}{2E_{\mathbf{k}+\mathbf{q}}}\frac{E_{\mathbf{k}+\mathbf{q}}(E_{\mathbf{k}+\mathbf{q}}+q_0)+\mathbf{k}(\mathbf{k}+\mathbf{q})+m^2}{(E_{\mathbf{k}+\mathbf{q}}+q_0)^2-E_{\mathbf{k}}^2}\frac{1}{e^{\beta(E_{\mathbf{k}+\mathbf{q}}-\mu)}+1} \\
&+\frac{1}{2E_{\mathbf{k}+\mathbf{q}}}\frac{E_{\mathbf{k}+\mathbf{q}}(E_{\mathbf{k}+\mathbf{q}}-q_0)+\mathbf{k}(\mathbf{k}+\mathbf{q})+m^2}{(E_{\mathbf{k}+\mathbf{q}}-q_0)^2-E_{\mathbf{k}}^2}\frac{1}{e^{\beta(E_{\mathbf{k}+\mathbf{q}}+\mu)}+1} \\
=& \frac{1}{2E_{\mathbf{k}}}[f(q_0)+f(-q_0)]N_F(E_{\mathbf{k}})
\end{aligned} \tag{9}
$$

Where we have defined

$$
f(q_0) = \frac{E_{\mathbf{k}}(E_{\mathbf{k}}-q_0)+\mathbf{k}(\mathbf{k}+\mathbf{q})+m^2}{(E_{\mathbf{k}}-q_0)^2-E_{\mathbf{k}+\mathbf{q}}^2}
$$

$$N_F(E_{\mathbf{k}}) = \frac{1}{e^{\beta(E_{\mathbf{k}}+\mu)}+1} + \frac{1}{e^{\beta(E_{\mathbf{k}}-\mu)}+1}$$

For vacuum part where we obtained in last section, it describes the intrinsic graphene, in which the conduction band is empty while the valence band is fully occupied at zero temperature. When $m \to 0$ graphene varies from a insulator to the zero-gap semiconductor system. When we take into account the finite density effect, the Fermi energy could lie either in valence band ($\mu < 0$) or in conduction band($\mu > 0$)

$$\begin{aligned} \Pi_{matter} &= 8\int \frac{d^2\mathbf{k}}{(2\pi)^2}\frac{1}{2E_{\mathbf{k}}}[f(q_0)+f(-q_0)]\Theta(E_{\mathbf{k}}-\mu) \\ &= \frac{1}{\pi^2}Re\int_0^{k_F}\frac{dkk}{E_{\mathbf{k}}}\int_{-1}^{1}dx\frac{1}{\sqrt{1-x^2}}(\frac{4E_{\mathbf{k}}^2-4q_0E_{\mathbf{k}}+q_0^2-q^2}{q_0^2-2q_0E_{\mathbf{k}}-q^2-2kqx}-1) \end{aligned} \tag{10}$$

The retarded polarization function of the free fermions

$$\Im m\Pi^{ret}_{matter} = \frac{1}{\pi}Re\int_0^{k_F}\frac{dkk}{E_{\mathbf{k}}}\int_{-1}^{1}dx\frac{4E_{\mathbf{k}}^2-4q_0E_{\mathbf{k}}+q_0^2-q^2}{\sqrt{1-x^2}}\delta(q_0^2-2q_0E_{\mathbf{k}}-q^2-2kqx) \tag{11}$$

And in the above equations, we have defined

$$Ref(q_0) = [f(q_0)+f(-q_0)]/2, Re\delta(f(q_0)) = [\delta(f(q_0))-\delta(f(-q_0))]/2$$

If we set $m = 0$, we calculate explicitly and find they just coincide with the Ref.[4][5], and its finite temperature counterparts were discussed in Ref.[6][7] while we emphasize that within our model we do not need the overlapping factor used in their work and the results come out more naturally.

$$\Im m\Pi^{ret}_{matter} = \frac{1}{\pi}Re\int_0^{k_F} dk\int_{-1}^{1}dx\frac{4k^2-4kq_0+q_0^2-q^2}{\sqrt{1-x^2}}\delta(q_0^2-2kq_0-q^2-2kqx) \tag{12}$$

$$\begin{aligned} \Im m\Pi^{ret}_{matter} &= \frac{1}{\pi}\int_0^{k_F} dk[\frac{(q_0-2k)^2-q^2}{q^2-q_0^2}]^{\frac{1}{2}}\{\Theta(q-q_0)\Theta(k-\frac{q+q_0}{2}) \\ &+\Theta(q_0-q)[\Theta(\frac{q_0+q}{2}-k)-\Theta(\frac{q_0-q}{2}-k)]\} \\ &-\frac{1}{\pi}\int_0^{k_F} dk[\frac{(q_0+2k)^2-q^2}{q^2-q_0^2}]^{\frac{1}{2}}\Theta(q-q_0)\Theta(k-\frac{q-q_0}{2}) \end{aligned} \tag{13}$$

$$\Pi^{ret}_{matter} = \Theta(q_0-q)\Pi_1^+ + \Theta(q-q_0)\Pi_2^+ \tag{14}$$

$$\begin{aligned} \Im m\Pi_1^+ &= -\frac{1}{2\pi\sqrt{q_0^2-q^2}}\{(2k_F-q_0)\sqrt{q^2-(2k_F-q_0)^2}+q^2\arcsin(\frac{2k_F-q_0}{2k_F})\Theta(q-|q_0-2k_F|) \\ &+ \frac{\pi q^2}{2}[\Theta(2k_F-q_0-q)+\Theta(2k_F-q_0+q)]\} \end{aligned} \tag{15}$$

$$\begin{aligned} \Im m\Pi_2^+ &= \frac{\Theta(2k_F+q_0-q)}{2\pi\sqrt{q^2-q_0^2}}\{(2k_F+q_0)\sqrt{(2k_F+q_0)^2-q^2}-q^2\ln\frac{\sqrt{(2k_F+q_0)^2-q^2}+2k_F+q_0}{q} \\ &- [(2k_F-q_0)\sqrt{(2k_F-q_0)^2-q^2}-q^2\ln\frac{\sqrt{(2k_F-q_0)^2-q^2}+2k_F-q_0}{q}]\Theta(2k_F-q_0-q)\} \end{aligned} \tag{16}$$

The real part can be obtained using Kramers-Kronig relation

$$\Re e\Pi^{ret}_{matter} = \frac{1}{\pi}\int_{-\infty}^{\infty} dq_0' \frac{\Im m\Pi^{ret}_{matter}(q_0)}{q_0' - q_0} \tag{17}$$

For the massive case(gapped graphene), the explicit calculation of the polarization function is straightforward[13][14], so we just discuss an important static case $q_0 = 0$

$$\begin{aligned}
\Pi^{ret}_{matter}(\mathbf{q},0) &= \frac{2}{\pi^2}\int_0^{k_F}\frac{dkk}{E_{\mathbf{k}}}\int_{-1}^{1}dx\frac{1}{\sqrt{1-x^2}}(\frac{q^2-4E^2_{\mathbf{k}}}{q^2+2kqx}-1) \\
&= -\frac{2}{\pi}(\sqrt{k_F^2+m^2}-\sqrt{m^2}) \\
&\quad +\frac{2}{\pi q}\int_0^{k_F}\frac{dkk}{\sqrt{k^2+m^2}}(\sqrt{q^2-4k^2}-4m^2/\sqrt{q^2-4k^2})\Theta(\frac{q}{2}-k) \\
&= -\frac{2}{\pi}(\mu-m) \\
&\quad +\frac{2}{\pi q}\int_m^{\mu}d\epsilon(\sqrt{q^2+4m^2-4\epsilon^2} \\
&\quad -4m^2/\sqrt{q^2+4m^2-4\epsilon^2})\Theta(\sqrt{q^2+4m^2}-2\epsilon)
\end{aligned} \tag{18}$$

$$\begin{aligned}
&\frac{2}{\pi q}\int_m^{\mu}d\epsilon(\sqrt{q^2+4m^2-4\epsilon^2}-4m^2/\sqrt{q^2+4m^2-4\epsilon^2})\Theta(\sqrt{q^2+4m^2}-2\epsilon) \\
= \;&\frac{1}{\pi q}\{[-mq+\frac{q^2-4m^2}{2}\arctan\frac{q}{2m}]\Theta(2k_F-q) \\
&+[\mu\sqrt{q^2-4k_F^2}-mq-\frac{q^2-4m^2}{2}\arctan\frac{\sqrt{q^2-4k_F^2}}{2\mu}+\frac{q^2-4m^2}{2}\arctan\frac{q}{2m}]\Theta(q-2k_F)\}
\end{aligned} \tag{19}$$

IV. STATIC SCREENING

The static screening properties of the massive Dirac fermions in the RPA are controlled by the static dielectric function $\varepsilon_{RPA}(q,0)$.

$$\varepsilon_{RPA}(q,0) = 1 - \frac{2\pi e^2}{\kappa q}[\Pi_{vac}(\mathbf{q},0)+\Pi_{matter}(\mathbf{q},0)] \tag{20}$$

Without the matter contribution, the polarized charge distribution has been discussed in Ref.[12] ,if we take into account the matter part, things will be quite different

For $q \le 2k_F$

$$\Pi(\mathbf{q},0) = -\frac{2\mu}{\pi} \tag{21}$$

For$q > 2k_F$

$$\Pi(\mathbf{q},0) = -\frac{2\mu}{\pi}+\frac{1}{\pi q}\Theta(q-2k_F)[\mu\sqrt{q^2-4k_F^2}-\frac{q^2-4m^2}{2}\arctan\frac{\sqrt{q^2-4k_F^2}}{2\mu}] \tag{22}$$

Similar results has been obtained in Ref.[15]. From above we can deduce that the density of state at the Fermi surface is given by $D(k_F) = 2\mu/\pi$, In the two limiting cases, the total static polarizability becomes a constant as in normal 2D electron liquid systems and 2D massless Dirac fermion systems. For 2D electron liquid, the 2D Thomas-Fermi wave vector is given by $q_{TF} = me^2/\kappa$. Consider a external charge density embedded in the homogeneous fermions.Even though $V_{ei}(\mathbf{x}) = C\delta(\mathbf{x})$ is short-ranged, the density response is not short-ranged which can be calculated by linear response theory[16].

$$\Pi(\mathbf{x}) = C\int \frac{d^2\mathbf{q}}{(2\pi)^2}\Pi(\mathbf{q},0)e^{i\mathbf{q}\cdot\mathbf{x}} \tag{23}$$

It is interesting to note that as the normal 2D electron liquid, the 2D Dirac fermions also has an oscillatory term due to the non-analyticity at $q = k_F$. Next, we take into account finite temperature dependant screening, the polarization function at $T \neq 0$ is

$$\begin{aligned}\Pi^{ret}_{matter}(\mathbf{q},T) = &-\frac{2}{\pi}\{\mu - m + \frac{1}{\beta}\ln[1+e^{-\beta(\mu-m)}] + \frac{1}{\beta}\ln[1+e^{-\beta(\mu+m)}]\}\\ &+\frac{2}{\pi q}\int_m^{\epsilon_{q/2}} d\epsilon (2\sqrt{\epsilon^2_{q/2}-\epsilon^2} - 2m^2/\sqrt{\epsilon^2_{q/2}-\epsilon^2})[\frac{1}{1+e^{\beta(\epsilon-\mu)}} + \frac{1}{1+e^{\beta(\epsilon+\mu)}}]\end{aligned} \tag{24}$$

At low temperature ($T \ll T_F$),we have the asymptotic from of the polarizability from the above equation

$$\Pi(\mathbf{q},T) \approx -\frac{2\mu(T)}{\pi} \quad \text{for} \quad \epsilon_{q/2} < \mu, \tag{25}$$

In particular, for $q = 2k_F$, $m \to 0$, we have

$$\begin{aligned}\Pi^{ret}_{matter}(\mathbf{q},T) = \quad & -\frac{2}{\pi}\{\mu + \frac{1}{\beta}\ln[1+e^{-\beta\mu}] + \frac{1}{\beta}\ln[1+e^{-\beta\mu}]\}\\ & + \frac{4}{\pi q}\int_0^{\epsilon_{q/2}} d\epsilon\sqrt{\epsilon^2_{q/2}-\epsilon^2}[\frac{1}{1+e^{\beta(\epsilon-\mu)}} + \frac{1}{1+e^{\beta(\epsilon+\mu)}}]\\ \approx \quad & -\frac{2}{\pi}\mu(T) + \frac{2k_F}{\pi}\int_0^1 dx\sqrt{1-x^2}(1 - e^{\beta(k_F x-\mu)} + e^{2\beta(k_F x-\mu)} + ...)\\ \approx \quad & -\frac{2}{\pi}\mu(T) + \frac{k_F}{2} - \sqrt{\frac{2}{\pi k_F}}(1-\frac{\sqrt{2}}{2})\zeta(\frac{3}{2})T^{3/2}\end{aligned} \tag{26}$$

And the total polarization function is

$$\Pi(\mathbf{q},T) \approx -\frac{2}{\pi}\mu(T) - \sqrt{\frac{2}{\pi k_F}}(1-\frac{\sqrt{2}}{2})\zeta(\frac{3}{2})T^{3/2} \tag{27}$$

While for a general m, analytic expressions can not be obtained, however, it is quite easy to obtain numerical results from our semi-analytical results.

At high temperature ($T \gg T_F$)

$$\Pi(\mathbf{q},T) \approx \frac{2}{\pi}\mu(T) + \frac{1}{\pi T}[\frac{q^2}{12} - m^2] \tag{28}$$

For the chemical potential $\mu(T)$, we can get its explicit form the conservation of the total electron density. For the massless Dirac fermions, the asymptotic expression has been given in Ref.[17]. We note that for the massive case the expressions is the same.

V. CONCLUSION

In summary, we have presented a finite temperature field model for the 2D massive Dirac fermions and calculated the polarization functions for massive Dirac fermions. Finite temperature and finite density were taken into account to analyze the physics of gapped graphene in a more general case and connect various other group's important work[4][5][6][7] done before. These results may be useful to study finite-temperature screening within the RPA. Other important quantities, for example conductivity or specific heat, can be obtain from our results.

The polarization function at finite temperature can be also used to calculate the thermodynamic properties of massive Dirac fermion.

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